LA-UR-20-23438

Title: Machine Learning for Memory Reduction in the Implicit Monte Carlo Simulations of Thermal Radiative Transfer

Author(s): Matsekh, Anna M.
Chacon, Luis
Park, HyeongKae
Chen, Guangye

Intended for: Report

Issued: 2020-05-07

Machine Learning for Memory Reduction in the Implicit Monte Carlo Simulations of Thermal Radiative Transfer

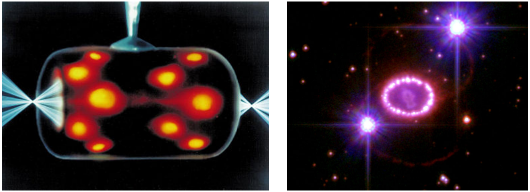
Anna Matsekh (CCS-2)
Luis Chacon (T-5), HyeongKae Park (T-3), Guangye Chen (T-5)

Los Alamos National Laboratory

Thermal Radiative Transfer

- *Thermal Radiative Transfer (TRT) equations*
  - describe propagation and interaction of photons with the surrounding material
  - are challenging to solve due to the stiff non-linearity and high-dimensionality of the problem

- *TRT applications at LANL include simulations of*
  - Inertial Confinement Fusion (ICF) experiments
  - astrophysical phenomena, such as collapsing stars



(a) ICF (b) supernova

Figure: TRT applications

Implicit Monte Carlo Simulations

- *Advantages, compared to the deterministic case*
  - easier to extend to complex geometries and higher dimensions
  - easier to parallelize
- *Disadvantages*
  - Monte Carlo solutions to IMC equations exhibit statistical variance and IMC convergence rate is estimated to be

$$O(1/\sqrt{N_p})$$

    where N_p is the number of simulation particles
  - Even when advanced variance reduction techniques employed, Monte Carlo simulations
    - require a very large number of simulation particles
    - exhibit slow convergence
    - prone to statistical errors
  - Implicit Monte Carlo codes are typically very large, long running codes with large memory requirements at checkpointing & restarting

Machine Learning for IMC

Project Goal: use parametric Machine Learning methods in order to reduce memory requirements at checkpointing & restarting in the IMC simulations of Thermal Radiative Transfer using

- *Expectation Maximization and Weighted Gaussian Mixture Model-based approach for 'particle-data compression', introduced in Plasma Physics to model Maxwellian particle distributions by Luis Chacon and Guangye Chen*
- *Expectation Maximization with Weighted Hyper-Erlang Model in order to compress isotropic IMC particle data in the frequency domain*
- *Expectation Maximization and von Mises-Fisher Mixture Model for compression of anisotropic IMC particle data in the angular domain (work-in-progress)*

Note: weighted Gaussian mixture models have been used at LANL in the simulations of radiographic X-ray sources (see 'A maximum likelihood method for linking particle-in-cell and Monte-Carlo transport simulations', Kevin J. Bowers, Barbara G. Devolder, Lin Yin, Thomas J.T. Kwan, (2004)).

TRT Equations

Consider 1-d Transport Equation without physical scattering and external sources, in the Local Thermodynamic Equilibrium (LTE):

$$\frac{1}{c}\frac{\partial I_\nu}{\partial t} + \mu\frac{\partial I_\nu}{\partial x} + \sigma_\nu\, I_\nu = \frac{1}{2}\,\sigma_\nu\, B_\nu \tag{1}$$

coupled to the Material Energy Equation

$$c_v\,\frac{\partial T}{\partial t} = \iint \sigma_\nu\, I_\nu\,\mathrm{d}\nu\,\mathrm{d}\mu - \int \sigma_\nu\, B_\nu \mathrm{d}\nu \tag{2}$$

where the emission term

$$B_\nu(T) = \frac{2\,h\,\nu^3}{c^2}\,\frac{1}{e^{\frac{h\,\nu}{k\,T}} - 1} \tag{3}$$

is the Planckian (Blackbody) distribution and

- $I_\nu = I(x, \mu, t, \nu)$ - radiation intensity
- ν - frequency, T - temperature
- σ_ν - opacity, c_v - material heat capacity
- k - Boltzmann constant, h - Planck's constant, c - speed of light

LDG-based Deterministic Solution

Backward-Euler discretization in time

$$\frac{1}{c}\,\frac{I^{(n+1)}-I^{(n)}}{\Delta t_n}+\mu\,\frac{\partial}{\partial x}I^{(n+1)}+\sigma\,I^{(n+1)}=\frac{1}{2}\,\sigma\,a\,c\,{T^{(n+1)}}^4 \tag{4}$$

Linear Discontinuous Galerkin (LDG) discretization, with basis functions defined in spacial cells $i=1,\ldots,n_c$:

$$\begin{aligned} I(x,\mu,t) &= I^0\,\phi_0(x)+I^1\,\phi_1(x) \\ \phi_0(x)=(x_{i+1/2}-x)/\Delta x, &\quad \phi_1(x)=(x-x_{i-1/2})/\Delta x \end{aligned} \tag{5}$$

Discrete Ordinates (Sn) discretization in angle $\mu=\mu_m$

$$E(x,t)=\frac{1}{c}\sum_m \omega_m\,(I_m^0\,\phi_0(x)+I_m^1\,\phi_1(x)) \tag{6}$$

where ω_m are the Gauss-Legendre quadrature weights

Temperature term $\Theta=a\,T^4$ can be represented as follows

$$\Theta(x,t)=\Theta^0\,\phi_0(x)+\Theta^1\,\phi_1(x) \tag{7}$$

Discretization of the Material Energy Equation

With Backward-Euler discretization in time

$$\rho\, c_\nu\, \frac{{T^i}^{(n+1)} - {T^i}^{(n)}}{\Delta t} + \sigma\, a\, c\, {T^i}^{(n+1)^4} - \sigma\, c\, E^i = 0, \quad i = 0, 1 \qquad (8)$$

and the following representation of temperature

$$T(x,t) = T^0 \phi_0(x) + T^1 \phi_1(x) \qquad (9)$$

We obtain a non-linear system of equations that can be solved via the Newton's Iteration in this simple case

$$\begin{cases} T^{(k+1)} = T^{(k)} + \delta T^{(k)}, \quad \delta T^{(k)} = -\dfrac{\mathcal{F}(T^{(k)})}{\mathcal{F}'(T^{(k)})} \\ \mathcal{F}(T^{(k)}) = \rho\, c_\nu\, \dfrac{T^{(k)} - T^{(k-1)}}{\Delta t} + \sigma\, a\, c\, {T^{(k)}}^4 - \sigma\, c\, E \\ \mathcal{F}'(T^{(k)}) = \dfrac{\rho\, c_\nu}{\Delta t} + 4\, \sigma\, a\, c\, {T^{(k)}}^3 = 0. \end{cases} \qquad (10)$$

Implicit Monte Carlo Method of Fleck and Cummings

Transport Equation

$$\frac{1}{c}\frac{\partial I_\nu}{\partial t} + \mu\frac{\partial I_\nu}{\partial x} + (\sigma_{\nu a} + \sigma_{\nu s})\, I_\nu = \frac{1}{2}\,\sigma_{\nu a}\, c\, u_r^n + \frac{1}{2}\,\sigma_{\nu s}\,(b_\nu/\sigma_p)\iint \sigma_{\nu'}\, I_{\nu'}\,\mathrm{d}\nu'\,\mathrm{d}\mu \tag{11}$$

Material Temperature Equation $(T^n = T(t_n) \approx T(t),\ t_n \leq t \leq t_{n+1})$

$$c_\nu\, T^{n+1} = c_\nu\, T^n - f\,\sigma_p\, c\,\Delta t\, u_r^n + f\int_{t_n}^{t_{n+1}}\mathrm{d}t\iint \sigma_{\nu'}\, I_{\nu'}\,\mathrm{d}\nu'\,\mathrm{d}\mu \tag{12}$$

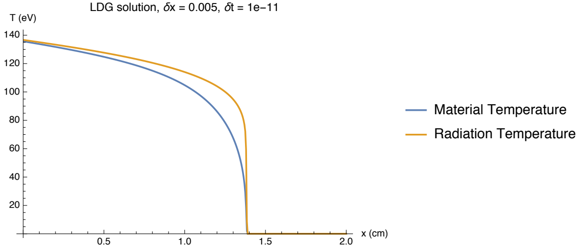
- $f = 1/(1 + \alpha\,\beta\, c\,\Delta t\,\sigma_p)$ - *Fleck factor*
- $\sigma_{\nu a} = f\,\sigma_\nu$ - *effective absorption opacity*
- $\sigma_{\nu s} = (1-f)\,\sigma_\nu$ - *effective scattering opacity*
- u_r - *radiation energy density*, $b_\nu(T)$ - *normalized Planckian*
- $\sigma_p = \int \sigma_\nu\, b_\nu\, d\nu$ - *Planck opacity*
- $\alpha \in [0,1]$ $s.t.$ $u_r \approx \alpha\, u_r^{n+1} + (1-\alpha)\, u_r^n; \beta = \partial u_r/\partial u_m$

Monte Carlo Implementation of the IMC method

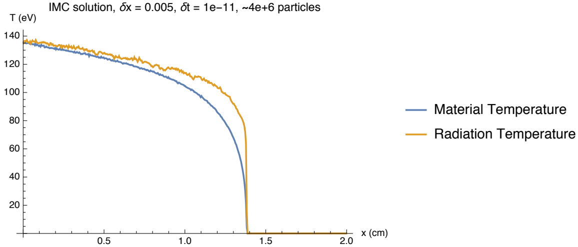
On each simulation time step

- *Particle Sourcing* – calculating total energy in the system from different sources due to the
    - boundary conditions and initial conditions
    - external sources and emission sources
- *Particle Tracking* – tracking distance to an event in time:
    - distance to the spacial cell boundary
    - distance to the end of the time-step
    - distance to the next collision
- *Tallying* - computing sample means of such quantities as
    - energy deposited due to all effective absorptions
    - volume-averaged energy density
    - fluxes
- *Calculate next time-step temperature approximation* T^{n+1}

1-d Gray Marshak Wave Problem



(a) LDG solution in slab geometry



(b) IMC solution in slab geometry

The concept of an IMC particle

- An IMC particle is a simulation abstraction representing a 'radiation energy bundle' characterized by
  - the energy-weight (*relative number of photons represented by an IMC particle*)
  - spacial location
  - angle of flight
  - frequency group it belongs to
- On each simulation time step $t_n \leq t \leq t_{n+1}$ an IMC particle can undergo the following events:
  - escape through the boundaries
  - get absorbed by the material
  - scattering / re-emission
  - survive (particle goes to census at t_{n+1})
- Surviving particles are called *census particles* and have to be stored in memory to be reused on the next time-step

Can we 'learn' the probability distribution function describing census particles at the end of each time-step and store in memory only this distribution?

Expectation Maximization Method

- *Expectation Maximization (EM) is an iterative method for estimating parameters from probabilistic models. It is typically applied to the Finite Mixture Models*

$$\mathcal{P}(x_j, \theta) = \sum_{i=1}^{k} p_i \, \mathcal{F}(x_j, \theta_i) \tag{13}$$

  - $\mathcal{F}(x_j, \theta_i)$ - *pdf* with the parameter vector θ_i
  - x_j - data points from the sample $X^n = (x_1, x_2, \ldots, x_n)$
  - p_i - probability of $\mathcal{F}(x_j, \theta_i)$ in the mixture $\sum_{i=1}^{n} p_i = 1$

- *EM algorithm alternates between the Expectation and Maximization steps:*
  - *Expectation (E) step - computing priors (probabilities)*
  - *Maximization (M) step - updating model parameters θ_i that maximize expected Likelihood function*

$$\mathcal{L}(X^n) = \sum_{j=1}^{n} \ln \sum_{i=1}^{k} p_i \, \mathcal{F}(x_j, \theta_i) \tag{14}$$

EM and Hyper-Erlang Model

- *A Hyper-Erlang Model* $\mathcal{H}(\nu, \alpha, \beta)$ is a mixture of Erlang distributions $\mathcal{E}(\nu, \alpha, \beta)$:

$$\sum_{k=1}^{m} p_k \, \mathcal{E}(\nu_i, \alpha_k, \beta_k) = \sum_{k=1}^{m} p_k \, \frac{1}{(\alpha_k - 1)!} \, \nu_i^{\alpha_k - 1} \, \beta_k^{-\alpha_k} \, e^{(-\nu_i/\beta_k)}$$

  where
  - $\{\nu_1, \ldots, \nu_n\}$ is an *iid* data sample
  - $\alpha_k > 0$ - integer *shape parameter*, $\beta_k > 0$ - real *scale parameter*
- *Expectation Maximization priors*

$$\gamma_{ik} = \frac{p_k \, \mathcal{E}(\nu_i, \alpha_k, \beta_k)}{\sum_{k=1}^{m} p_k \, \mathcal{E}(\nu_i, \alpha_k, \beta_k)}, \quad i = 1, \ldots, n, \;\; k = 1, \ldots m \quad (15)$$

- *Maximum Likelihood parameter estimates*

$$\beta_k = \frac{\sum_{i=1}^{n} \gamma_{ik} \, \nu_i}{\alpha_k \, \sum_{i=1}^{n} \gamma_{ik}}, \quad p_k = \frac{\sum_{i=1}^{n} \gamma_{ik}}{n}, \;\; k = 1, \ldots, m \qquad (16)$$

Planckian and Erlang Distributions

- *In the LTE emission term in the Transport Equation is given by the Planckian B_ν*
- *Frequency-normalized Planckian density function*

$$b_\nu(T) = \frac{B_\nu(T)}{\int_0^\infty B_\nu(T)d\nu} = \frac{15}{\pi^4}\,\frac{\nu^3}{T^4\,(e^{\nu/T}-1)} \tag{17}$$

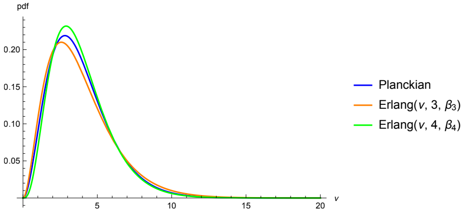
- *There are no closed-form EM estimates of T for $b_\nu(T)$ mixtures*
- *Can we model Planckian-like distributions with Erlang mixtures?*
    - Erlang distribution

$$\mathcal{E}(\nu,\alpha,T) = \frac{1}{(\alpha-1)!}\,\frac{\nu^{\alpha-1}}{T^\alpha\,e^{\nu/T}} \tag{18}$$

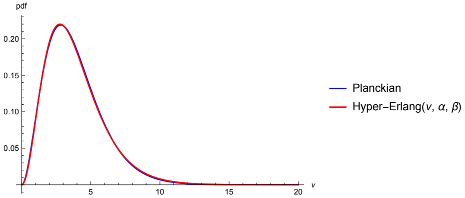
    - Consider Erlang distributions with shapes $\alpha = \{3,4\}$

$$\mathcal{E}(\nu,3,T) = \frac{1}{2}\,\frac{\nu^2}{T^3\,e^{\nu/T}},\quad \mathcal{E}(\nu,4,T) = \frac{1}{6}\,\frac{\nu^3}{T^4\,e^{\nu/T}} \tag{19}$$

Planckian and Erlang Distributions



(a) Planckian and Erlang pdf



(b) Hyper-Erlang pdf ($\alpha = \{3, 4\}$-mixture)

Figure: Planckian frequency data sample size: $200,000$

Hyper-Erlang Model for IMC

- IMC particles in group g are characterized by the same average frequency, i.e. have the same likelihood to be drawn from g
- Cumulative energy-weight $\omega^g = \sum_{j=1}^{np_g} \omega_j^g$ of np_g particles in g is the relative number of photons represented by all particles in g
- *Weighted Log-Likelihood of the Hyper-Erlang IMC Model*

$$\ln \prod_{g=1}^{n} \left(\sum_{k=1}^{m} p_k \, \mathcal{E}(\nu_g, \alpha_k, \beta_k) \right)^{\omega^g} = \sum_{g=1}^{n} \omega^g \ln \sum_{k=1}^{m} p_k \, \mathcal{E}(\nu_g, \alpha_k, \beta_k)$$

- *Weighted Maximum Likelihood / EM parameter estimates*

$$\gamma_{gk} = \frac{p_k \, \mathcal{E}(\nu_g, \alpha_k, \beta_k)}{\sum_{k=1}^{m} p_k \, \mathcal{E}(\nu_g, \alpha_k, \beta_k)}, \quad g = 1, \ldots, n, \;\; k = 1, \ldots m$$

$$\beta_k = \frac{\sum_{g=1}^{n} \omega^g \, \gamma_{gk} \, \nu_g}{\alpha_k \, \sum_{g=1}^{n} \omega^g \, \gamma_{gk}}, \quad p_k = \frac{\sum_{g=1}^{n} \gamma_{gk}}{\sum_{g=1}^{n} \omega^g}$$

Weighted Hyper-Erlang Model for compressing IMC particles

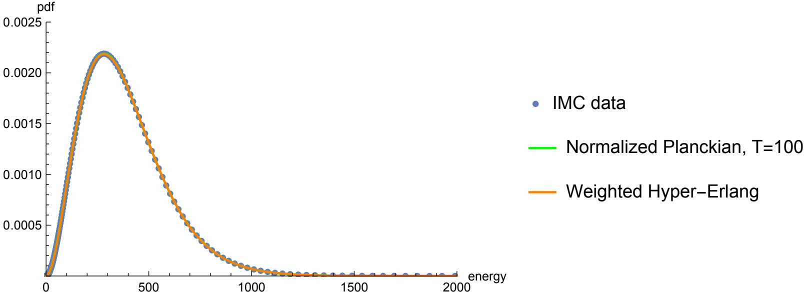


Figure: Planckian IMC data sample from the time step $t_0 = 0$ (initial temperature $T_0 = 100$, 500 groups), Normalized Planckian $b_\nu(T)$ at $T = 100$ and the Hyper-Erlang Model $\mathcal{H}(\nu, \alpha, \beta)$ of the sample with 20 mixture elements.

Note: for $\mathbf{x} \sim b_\nu(T)$ and $\mathbf{y} \sim \mathcal{H}(\nu, \alpha, \beta)$: $\|\mathbf{x} - \mathbf{y}\|_\infty = 6.2 \times 10^{-6}$

Weighted Hyper-Erlang Model

Table: Parameters of the Hyper-Erlang Model of the Planckian IMC data sample with initial temperature $T_0 = 100$ from the time step $t_0 = 0$. Shape parameters α_k are fixed, scale parameters β_k model radiation temperature and $k = 1, 2, \ldots, 20$.

p_k	α_k	β_k
0.	1	358.246
0.0248371	2	182.592
0.2026990	3	97.1897
0.2191770	4	71.5419
0.1673600	5	73.3836
0.1283270	6	69.3727
0.0927585	7	64.5944
0.0622957	8	61.4264
0.0394477	9	60.4135
0.0244054	10	60.7461
0.0151412	11	61.0587
0.0094205	12	60.8283
0.0058112	13	59.8523
0.0035262	14	58.2133
0.0020989	15	56.3901
0.0012253	16	54.7773
0.0007035	17	53.6442
0.0004003	18	53.2266
0.0002299	19	53.6196
0.0001359	20	54.2246

Compression of directional data

- von Mises-Fisher distribution on a sphere in $\mathbb{R}^p$:

$$\mathcal{MF}(\mathbf{x},\, \lambda,\, \kappa) = \frac{\kappa^{p/2-1}}{(2\,\pi)^{p/2}\, I_{p/2-1}(\kappa)}\, e^{\kappa\,(\lambda^{\mathsf{T}}\,\mathbf{x})} \tag{20}$$

  - $\mathbf{x} \in \mathbb{R}^p,\ \|\mathbf{x}\| = 1$ - random vector
  - $\lambda,\ \|\lambda\| = 1$ - mean direction parameter vector
  - $\kappa \geq 0$ - the concentration parameter
  - $I_n(\kappa)$ - the modified Bessel function of the first kind of order n

- von Mises (Tikhonov / Circular Normal) distribution on a circle for random angle $\theta \in [0, 2\,\pi)$

$$\mathcal{M}(\theta,\, \phi,\, \kappa) = \frac{e^{\kappa\, \cos\,(\theta-\phi)}}{2\,\pi\, I_0(\kappa)} \tag{21}$$

where mean angle $\phi \in [0, 2\,\pi)$ and concentration $\kappa \geq 0$.

  - when concentration $\kappa = 0$, $\mathcal{M}(\theta,\, \phi,\, \kappa)$ is isotropic in angle
  - the larger is κ, the more concentrated is $\mathcal{M}(\theta,\, \phi,\, \kappa)$ around ϕ

von Mises distribution on a circle

$$\mathcal{M}(\theta,\,\phi,\,\kappa) = \frac{e^{\kappa\ \cos(\theta-\phi)}}{2\,\pi\,I_0(\kappa)}$$

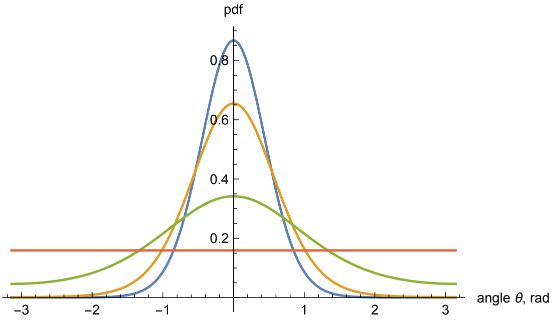


Figure: Probability density function of the von Mises distribution for the angle $\theta \in [-\pi, \pi]$ and mean angle $\phi = 0$

MLE parameter estimation for von Mises distribution

Consider angular data sample

$$(\theta_1, \ldots, \theta_n).$$

Let $s = \sum_i^n \sin\theta_i, \quad c = \sum_i^n \cos\theta_i$. Then the MLE of the mean angle ϕ is defined as follows:

$$\phi = \begin{cases} \arctan(s/c), \quad c > 0, s \geq 0 \\ \arctan(s/c) + 2\,\pi, \quad c > 0, s < 0 \\ \pi/2, \quad c = 0, s > 0, \quad 3\,\pi/2 \quad c = 0, s \leq 0 \\ \arctan(s/c) + \pi, \quad c < 0 \end{cases} \tag{22}$$

The MLE of the concentration κ can be approximated as follows:

$$\kappa \approx \begin{cases} 2.0\,R + R^3 + 0.83\,R^5, \; R < 0.53 \\ -0.4 + 1.39\,R + 0.43/(1.0 - R), \; 0.53 < R < 0.85 \\ 1/(R^3 - 4.0\,R^2 + 3\,R), \; R > 0.85, \end{cases}$$

where $R = \sqrt{s^2 + c^2}/n$ is the normalized resultant (*Fisher, 1993*).

Expectation Maximization for von Mises Mixtures

If we define 'mixture sin' and 'mixture cos'

$$\tilde{s}_k = \sum_{i=1}^{n} \gamma_{ik} \sin\theta_i, \qquad \tilde{c}_k = \sum_{i=1}^{n} \gamma_{ik} \cos\theta_i$$

we can rewrite EM estimates ϕ_k of the mean angle as follows:

$$\phi_k = \begin{cases} \arctan(\tilde{s}_k/\tilde{c}_k), & \tilde{c}_k > 0, \tilde{s}_k \geq 0 \\ \arctan(\tilde{s}_k/\tilde{c}_k) + 2\pi, & \tilde{c}_k > 0, \tilde{s}_k < 0 \\ \pi/2, \quad \tilde{c}_k = 0, \tilde{s}_k > 0, \quad 3\pi/2 & \tilde{c}_k = 0, \tilde{s}_k \leq 0 \\ \arctan(\tilde{s}_k/\tilde{c}_k) + \pi, & \tilde{c}_k < 0 \end{cases}$$

Expectation Maximization for von Mises Mixtures

We can now define 'normalized mixture resultant'

$$R_k = \frac{\sqrt{\tilde{s}_k^2 + \tilde{c}_k^2}}{\sum_{i=1}^{n} \gamma_{ik}}$$

'normalized mixture sin' and 'normalized mixture cos'

$$\sin\phi_k = \frac{\tilde{s}_k}{R_k}, \quad \cos\phi_k = \frac{\tilde{c}_k}{R_k}$$

and the mixture concentration parameter can now be estimated as

$$\kappa_k \approx \begin{cases} 2\,\mathcal{R}_k + \mathcal{R}_k^3 + \frac{5}{6}\,\mathcal{R}_k^5, \ \mathcal{R}_k < 0.53 \\ -0.4 + 1.39\,\mathcal{R}_k + 0.43/(1.0 - \mathcal{R}_k), \ 0.53 < \mathcal{R}_k < 0.85 \\ 1/(\mathcal{R}_k^3 - 4\,\mathcal{R}_k^2 + 3\,\mathcal{R}_k), \ \mathcal{R}_k > 0.85 \end{cases}$$

von Mises Mixture Model of isotropic angular IMC data

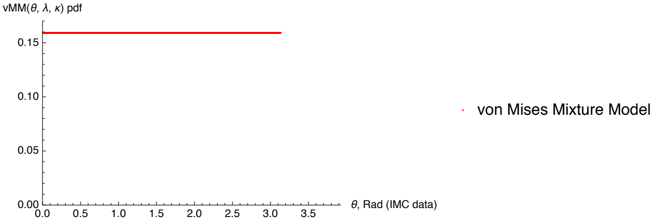


Figure: Angular IMC data distributed isotropically on [0, Pi], fitted to the learned 4-component von Mises Mixture Model

p_k	ϕ_k	κ_k
0.25	1.5667	0.0
0.25	1.5667	0.0
0.25	1.5667	0.0
0.25	1.5667	0.0

Table: Learned parameters of the 4-component von Mises Mixture Model. Log-likelihood error estimate $\delta = 9.3e - 10$.

von Mises Mixture Model of anisotropic angular IMC data

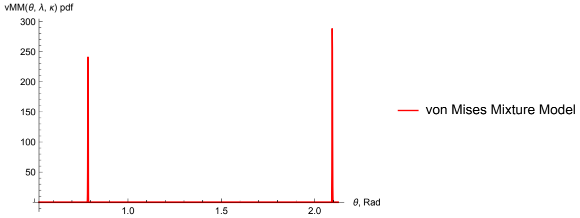


Figure: 4-component von Mises Mixture Model of IMC data equally concentrated around $\pi/4 \approx 0.785398$ and $2\,\pi/3 \approx 2.0944$ (estimates from the 15th EM iteration step)

p_k	ϕ_k	κ_k
0.47435413	0.785398	1493507.3
0.02537341	1.056737	3.68
0.02448313	1.784607	3.48
0.47578933	2.094395	2242910.4

Table: Parameters of the 4-component von Mises Mixture Model (estimates from the 15th EM iteration step)

Summary and Future Work

- *Memory usage reduction during the code checkpointing and restarting steps is of great importance in the IMC simulations*
- *Innovation: storing only parameters of the probability distributions of census particles in place of the data structures describing them in order to reduce IMC storage requirements*
- *Innovation: Expectation Maximization and Weighted Hyper-Erlang Models can accurately model Planckian and therefore are appropriate for compression of isotropic IMC census data in the frequency domain in LTE*
- *Innovation: We are currently researching applicability of the Expectation Maximization and von Mises-Fisher Mixture Models for compression of anisotropic IMC census data in angle*